Experimental Validation of the Crystal Lattice Model in the R-Matrix Code SAMMY

Arnaud Courcelle[1], Gilles Noguere[1], Nancy M. Larson[2]

[1] *CEA Cadarache*
[2] *Oak Ridge National Laboratory*

In the evaluation of low energy cross-sections, the broadening of neutron resonances due to the motion of the target nucleus at the atomic scale has been thorougly studied. The simplest model for Doppler Broadening is the Free Gas Model (**FGM**) that neglects atomic interaction between the target nuclei present in a sample. When the target atoms are bound to a molecule or a crystal, the incident neutron energy can change the atomic vibrational or rotational quantum state and a more realistic treatment is needed. Lamb [1] in the early days of cross-section theories derived a theoretical expression to account for the presence of chemical binding in a crystal sample. This model, known as the Crystal Lattice Model (**CLM**), accounts for the emission or absorption of phonon (quantum of vibrational energy) and expresses the capture cross-section as a function of the weighted spectrum of the lattice vibration frequencies.

This model was recently implemented in the bayesian R-matrix fitting computer code SAMMY [2]. SAMMY is widely used in the analysis and evaluation of cross-section data in the thermal, resolved and unresolved range. Based on the DOPUSH program [3], the phonon expansion method is used to compute the CLM Doppler broadening function.

In the present work, the Crystal Lattice Model of SAMMY is tested against transmission experiments performed at GELINA on U238 [4]. These experiments have been carried out to study Doppler broadening of neutron resonances at low temperature where the chemical binding effects can be easily detected. The measurements were performed with U and UO_2 samples at 23.7K and at room temperature. It is shown in this work that the Crystal Lattice Model of SAMMY well reproduces the assymetrical shape of the experimental transmission spectra in the vicinity of the 6.7 eV, 20.9 eV and 36.7 eV resonances. This paper also suggests several extensions in the present CLM model to remove some current approximations .

References

[1] W. E. Lamb, "Capture of neutrons by atoms in a crystal, " *Phys. Rev. 52, 295 (1937)*

[2] N. M. Larson, "Updated users' guide for SAMMY : Multilevel R-Matrix fits to neutron data using Bayes' equations, " *ORNL/TM-9179/R6 ENDF-364*

[3] D. Nabarejnev, Claude Mounier, Richard Sanchez, "The influence of crystalline binding on resonant absorption, " *Nuc. Sci. Eng. 131, 222-229 (1999)*

[4] A. Meister et al., "Experimental study of the Doppler broadening of neutron resonances at GELINA, " *Proc. Conf. Nuc. Data, Long Island, October 5-8, 1998*

Email: arnaud.courcelle@cea.fr